International Journal of Quantum Information

Three-spin interactions and entanglement in optical lattices

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The entanglement properties of some novel quantum systems are studied that are inspired by recent developments in cold-atom technology. A triangular optical lattice of two atomic species can be employed to generate a variety of spin-1/2 Hamiltonians including effective three-spin interactions. A variety of one or two dimensional systems can thus be realized that possess multi-degenerate ground states or non-vanishing chirality. The properties of these ground states and their phase transitions are probed with appropriate measures such as the entropic entanglement and the spin chirality.

Keywords: Entanglement; optical lattices.

1. Introduction

Since the development of optical lattice technology [1,2,3], considerable attention has been paid to the experimental simulation of a variety of condensed matter systems, such as spin chains [4,5,6,7], and to the realization of quantum computation [8]. Optical lattices allow to probe and realize complex quantum models with unique properties in the laboratory. Examples of particular interest in various areas of physics, are systems with many-body interactions. The latter have been hard to realize experimentally in the past due to the difficulty in controlling them externally or isolating them from the environment [9]. In contrast, optical lattices give the means to realize such interactions. Their long coherence times and their large degree of controllability that have been studied theoretically and experimentally [10,11,12] pave the way towards the observation of "higher order" phenomena. Their applications is of interest to cold atom technology as well as to condensed matter physics and quantum information.

As a concrete physical system we shall consider the case of two different atomic species, corresponding to different internal states of the atom, superposed by optical lattices. The latter are standing laser waves produced, for example, by a laser radiation trapped in an optical cavity. Each atom can be considered as a dipole that experiences the standing wave as a periodic sinusoidal potential. By employing two standing laser radiations which differ in polarization or frequency it is possible to trap the two different internal states of the atom and manipulate them individually.

For cold enough atoms and for sufficiently large amplitudes of the standing waves it is possible to bring the system to the Mott insulator phase where there is only one atom per site. This results in a two dimensional Hilbert space for each site spanned by the two possible states of an atom, namely $|\uparrow\rangle$ and $|\downarrow\rangle$, which effectively represent a spin-1/2 system.

Even if the number of atoms at each site is constant throughout the lattice there are still quantum effects present. They are mediated by virtual transitions dictated by the tunnelling from one site to its neighbor sites with coupling, J, and by collisions that take place when two or more atoms are located within the same site with coupling, U. The physical conditions of weak tunnelling couplings, $J \ll U$, and weak atomic densities assure that we are always in the Mott insulator regime with one atom per site. To analyze the evolution of the system we apply perturbation theory that restricts to the subspace of low energy states with one atom per site which are virtually interacting with the rest energetically unfavorable states. Considering up to the third order in perturbation theory it is shown that a triangular configuration of the lattice, as in Figure 1, results in a Hamiltonian that includes a variety of three-spin interactions. They arise from the possibility of atoms tunnelling along two different paths.

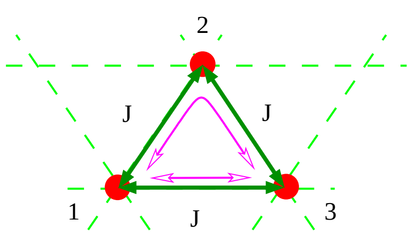

Fig. 1. The basic building block for the triangular lattice configuration. Three-spin interaction terms appear between sites 1, 2 and 3. For example, tunneling between 1 and 3 can happen through two different paths, directly and through site 2. The latter results in an exchange interaction between 1 and 3 that is influenced by the state of site 2.

Several applications spring out from our studies. The systematic description of the low energy Hamiltonian provides the means for the advanced control of the three-spin interactions simulated in the lattice. Hence, different physical models can be realized, with ground states that present a rich structure such as multiple degeneracies and a variety of quantum phase transitions [13,14,15]. Subsequently, these phases may also be viewed as possible phases of the initial atomic system, that is in the Mott insulator, where the behavior of the ground state can be controlled at will. These multi-particle interactions can be realized, in principle, with the near future technology.

2. Effective three-spin interactions

Consider the low energy evolution of the triangular system given in Figure 1 of three atoms in three sites of the lattice. By applying perturbation theory up to the third order we obtain the effective evolution of the system. As we restrict to the low energy space of states given by $|\uparrow\rangle$ and $|\downarrow\rangle$ for each site it is possible to express the effective Hamiltonian in terms of Pauli spin-1/2 operators explicitly given in the following

$$H_{eff} = \sum_{j=1}^{3} \Big[\; \mathbf{B}_j \cdot \boldsymbol{\sigma}_j + \lambda_j^{(1)} \sigma_j^z \sigma_{j+1}^z + \lambda_j^{(2)} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) \\ + \lambda^{(3)} \sigma_j^z \sigma_{j+1}^z \sigma_{j+2}^z + \lambda_j^{(4)} (\sigma_j^x \sigma_{j+1}^z \sigma_{j+2}^x + \sigma_j^y \sigma_{j+1}^z \sigma_{j+2}^y) \Big]. \qquad (1)$$

Up to the second order the Hamiltonian includes a Zeeman field, an Ising interaction and an XX interaction. The three-spin interactions presented in the last line can be viewed as the two spin interactions controlled by the third spin through an additional σ^z operator (see Figure 1). The couplings, $\mathbf{B}$ and $\lambda^{(i)}$, can be given as expansions in $J^\sigma/U_{\sigma\sigma'}$ where $\sigma =\uparrow, \downarrow$. These interactions can be straightforwardly extended to the case of a semi-one dimensional model (see Figure 2) or a two dimensional one.

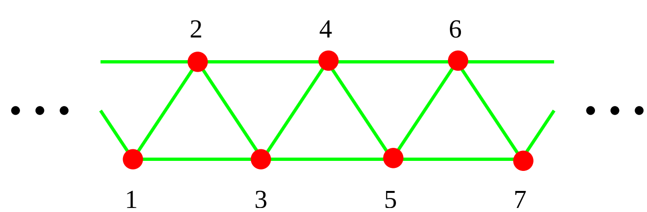

Fig. 2. The one dimensional chain constructed out of equilateral triangles. Each triangle experiences the three-spin interactions presented in the previous.

One can isolate different parts of the Hamiltonian (1), each one including a three-spin interaction term, by varying the tunnelling and/or the collisional couplings appropriately so that particular terms in considering up to the third order of the perturbation theory vanish, while others are freely varied. In particular, we would like to see if we can make the three-spin interaction dominating the two spin ones. Indeed, this is the case for particular values of J^σ and $U_{\sigma\sigma'}$ as we can see in Figure 3.

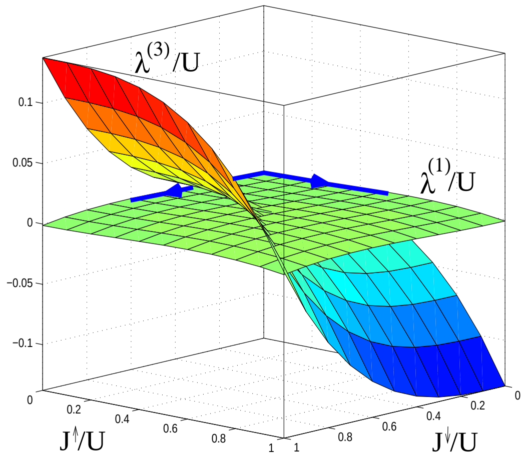

Fig. 3. The effective couplings $\lambda^{(1)}$ and $\lambda^{(3)}$ are plotted against $J^{\uparrow}/U$ and $J^{\downarrow}/U$ for $U_{\uparrow\uparrow} = U_{\downarrow\downarrow} = 2.12U$ and $U_{\uparrow\downarrow} = U$. The coupling $\lambda^{(1)}$ appears almost constant and zero as the unequal collisional terms can create a plateau area for a small range of the tunnelling couplings, while $\lambda^{(3)}$ can be varied freely to positive or negative values.

A particular example of a model that can be simulated in the optical lattice is described by the one dimensional Hamiltonian of the form

$$H(B_x, B_z) = -\sum_j \left(B_x \sigma_j^x + B_z \sigma_j^z + \sigma_j^z \sigma_{j+1}^z \sigma_{j+2}^z \right) \tag{2}$$

where all of its couplings can be arbitrarily and independently varied. The three-spin interaction term of this Hamiltonian possesses fourfold degeneracy in its ground state, spanned by the states $\{|\uparrow\uparrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle\}$. The criticality behavior of this model has been extensively studied in the past [16,17], where it is shown to present first and second order phase transitions. In particular, for $B_z = 0$ its self-dual character can be demonstrated [18,19]. To explicitly show that let us define the dual operators

$$\bar{\sigma}_j^x \equiv \sigma_j^z \sigma_{j+1}^z \sigma_{j+2}^z, \quad \bar{\sigma}_j^z \equiv \prod_{k=0}^{\infty} \sigma_{i-3k}^x \sigma_{i-3k-1}^x, \tag{3}$$

that also satisfy the usual Pauli spin-1/2 algebra. We can re-express the Hamiltonian $H(B_x, 0)$ with respect to the new operators obtaining finally

$$H(B_x, 0) = B_x H(B_x^{-1}, 0). \tag{4}$$

This equation of self-duality indicates that if there is one critical point then it should be at $|B_x| = 1$.

As it is not possible to explicitly solve the model we can employ numerical techniques to establish its criticality. For that, we shall consider an appropriate measure of entanglement, the entropy of entanglement [20], that successfully reveals the criticality behavior of our system. This measure is given by the von Neumann

entropy, S_L, of the reduced density matrix, ρ_L, of a subsystem of L successive spins analytically given by

$$S_L \equiv \mathrm{tr}(\rho_L \log \rho_L) \quad \text{with} \qquad \rho_L \equiv \mathrm{tr}_{N-L} |\psi\rangle\langle\psi| \tag{5}$$

where $|\psi\rangle$ is the total ground state. We know that for non-critical chains S_L should be saturated for large enough values of L. Indeed, this behavior is observed from the simulations when $B_x \neq 1$. On the other hand, when the system experiences second order criticality we expect $S_L \approx \frac{c+\bar{c}}{6} \log L$, where c is the central charge of the corresponding conformal field theory and $\bar{c}$ is its complex conjugate. The central charge uniquely corresponds to the critical exponents of the energy and of the correlation length, z and ν, respectively [13]. Indeed, at $B_x = 1$ we obtain Figure 4 that shows the expected logarithmic progression. By a logarithmic fitting we can deduce that $c \approx 4/5$, revealing that our model is in the same universality class as the three states Potts model with critical exponents $z = 1$ and $\nu = 3/4$.

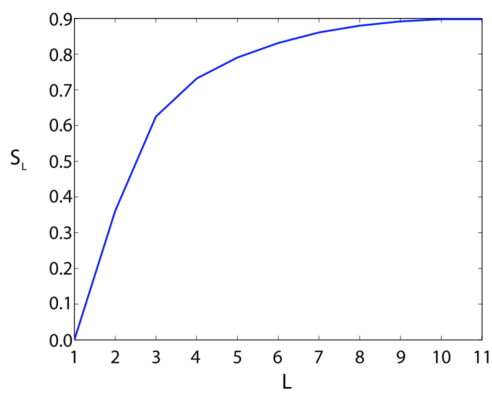

Fig. 4. Entropy of entanglement, S_L, as a function of L for a total of 19 spins. The plot shows a logarithmic behavior that indicates criticality for $B_x = 1$.

3. Complex tunnelling and topological effects

Consider the case where the tunnelling couplings in the setup described above are complex. This can be achieved by employing the electric moment $\mathbf{d}_e$ of the neutral atoms and an external magnetic field gradient. Without restrictions, we assume that the dipole is created out of two charges e and $-e$ at positions $\mathbf{x}$ and $\mathbf{x}+\mathbf{d}$, respectively, where $\mathbf{d}_e \equiv e\mathbf{d}$. Hence, its interaction with the field can be described by the minimal coupling

$$\begin{aligned}\mathbf{p} &\rightarrow \mathbf{p} + e\big[\mathbf{A}(\mathbf{x}+\mathbf{d}) - \mathbf{A}(\mathbf{x})\big] \\ &\approx \mathbf{p} + e\big[\mathbf{A}(\mathbf{x}) + (\mathbf{d}\cdot\boldsymbol{\nabla})\mathbf{A}(\mathbf{x}) - \mathbf{A}(\mathbf{x})\big] = \mathbf{p} + (\mathbf{d}_e\cdot\boldsymbol{\nabla})\mathbf{A}(\mathbf{x})\end{aligned} \tag{6}$$

where the limit of small $|\mathbf{d}|$ with respect to the variation of the magnetic field has been taken.

One can evaluate the phase produced by an electric dipole making a circular path in the presence of a magnetic field. Indeed, by employing Stokes's theorem we have

$$\phi = \oint_C (\mathbf{d}_e \cdot \boldsymbol{\nabla})(\mathbf{A}(\mathbf{x}) \cdot d\mathbf{l}) = \int\int_\Sigma (\mathbf{d}_e \cdot \boldsymbol{\nabla})(\mathbf{B} \cdot d\mathbf{S}) \tag{7}$$

where $d\mathbf{l}$ and $d\mathbf{S}$ are the line and surface elements, respectively.

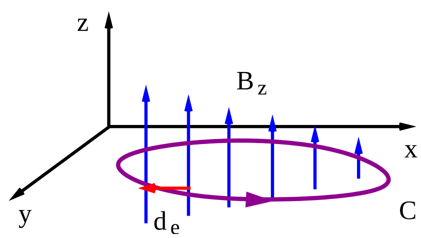

Fig. 5. A dipole circulating a magnetic field that has a constant gradient in the x-direction, while the field is homogenous in the y-direction. The resulting quantum phase is equivalent to having a charged particle circulating a homogeneous magnetic flux.

For example, consider the case of a magnetic field oriented along the z-direction with a non-vanishing gradient along the x-axis, as in Figure 5. Then for an electric dipole oriented along x, that performs a loop enclosing a surface Σ on the x-y plane, we have

$$\phi \ = \int\int_\Sigma d_e \frac{\partial B_z}{\partial x} dxdy = \int\int_\Sigma q^* B^* dxdy \tag{8}$$

where the effective charge and magnetic field are given by

$$q^* B^* = d_e \partial B_z / \partial x. \tag{9}$$

Hence, it is apparent that the phase obtained by a circulating dipole in the presence of a constant gradient of the magnetic field can actually simulate the effect of a circulating charge in a homogenous magnetic field. This analogy can be generalized to the case of many (neutral) particles in a superfluid phase such as a Bose-Einstein condensate. For the latter, an alternative way to simulate the effect of a charged particle in the presence of a magnetic field is given by just rotating it. Though, by employing present atom chip technology the gradient of a magnetic field can achieve $q^* B^*$ that is 10 to a 100 times stronger than the one obtained by the rotating technique.

Consider now the case where the atoms are superposed by optical lattices. If the dipole tunnels from one site to its neighboring one then there is a phase factor contribution to the tunnelling couplings, $J = e^{i\phi}|J|$, with

$$\phi = \int_{\mathbf{x}_i}^{\mathbf{x}_{i+1}} (\mathbf{d}_e \cdot \boldsymbol{\nabla})\mathbf{A} \cdot d\mathbf{x}. \tag{10}$$

Here $\mathbf{x}_i$ and $\mathbf{x}_{i+1}$ denote the positions of the lattice sites connected by the tunnelling coupling J. In order to isolate the additional terms that appear in the case of complex tunnelling couplings we should restrict ourselves to purely imaginary ones, i.e. we assume $J_j^\sigma = \pm i|J_j^\sigma|$. Then the effective Hamiltonian becomes

$$H_{eff} = \sum_i \Big[\ \mathbf{B} \cdot \boldsymbol{\sigma}_i + \tau^{(1)} \sigma_i^z \sigma_{i+1}^z + \tau^{(2)} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) \\ + \tau^{(3)} (\sigma_i^x \sigma_{i+1}^y - \sigma_i^y \sigma_{i+1}^x) + \tau^{(4)} \epsilon_{lmn} \sigma_i^l \sigma_{i+1}^m \sigma_{i+2}^n \Big], \tag{11}$$

where ϵ_{lmn} with $\{l, m, n\} = \{x, y, z\}$ denotes the total antisymmetric tensor in three dimensions and summation over the indices l, m, n is implied. The couplings $\tau^{(i)}$, appearing in (11) are functions of the original tunnelling and collisional couplings and can be varied at will. For example, by appropriately tuning J^a and U_{ab} and with the aid of compensating Zeeman terms we can set several of the $\tau^{(i)}$ couplings to zero obtaining the Hamiltonian

$$H_{eff} = \sum_i \Big[\tau^{(1)} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_{i+1} + \tau^{(4)} \boldsymbol{\sigma}_i \cdot (\boldsymbol{\sigma}_{i+1} \times \boldsymbol{\sigma}_{i+2}) \Big], \tag{12}$$

with $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$. The three-spin interaction term in (12) is also known in the literature as the chirality operator [21]. It breaks time reversal symmetry of the system as a consequence of the externally applied field. It is of great interest to study the ground state of this interaction in two dimensions, where states with solitonic character [21,22,23] are expected to form the ground states.

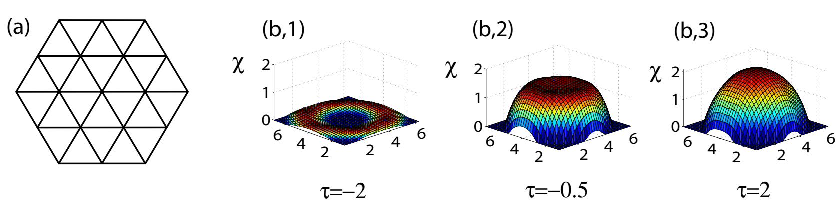

Fig. 6. (a) The hexagonal structure with 19 spins on the vertices and the 24 triangles. (b) The chirality, χ, as a function of the plaquette positioned on the plane for three different couplings τ. The generation of a localized skyrmion is apparent for large and positive values of τ.

As a particular example, for studying the behavior of this three-spin interaction term, we take a hexagonal configuration of 19 spin as in Figure 6(a). On this lattice we simulate Hamiltonian (12) for $\tau^{(1)} = \tau \cdot \tau^{(4)}$ with the additional condition that the spins on the boundary experience a strong magnetic field oriented in the z-direction. A numerical simulation has been performed to obtain the chirality of the ground state, $\chi \equiv \langle \vec{\sigma}_i \cdot \vec{\sigma}_j \times \vec{\sigma}_k \rangle$, for each triangular plaquette of neighboring sites i, j and k. In Figure 6(b) the chirality for different values of τ on the plane of the hexagon is given for three distinctive values of τ.

It is apparent that when τ is large and negative a ferromagnetic state is dominant that has zero chirality. On the other hand, when τ is large and positive frustration is dominating that cooperates with the chiral term for the generation of a chiral ground state. This is clearly indicated in Figure 6(b) where non-zero chirality is localized in the center of the hexagon indicating the presence of a skyrmion-like configuration.

To better understand the nature of the ground state we look at the possible expectation values the chirality operator can take for an arbitrary state of the spins on a certain triangle. It is easy to verify [24] that a product state gives $|\chi| \leq 1$, a bipartite entangled state gives $|\chi| \leq 2$, while states with $|\chi| > 2$ are necessarily tripartite entangled. From Figure 6(b) it is possible to see that this is the case for $\tau \approx 2$ indicating that the ground state at the center of the hexagon possesses tripartite entanglement.

4. Conclusions

In this article we presented a variety of different spin interactions that can be generated by a system of ultra-cold atoms superposed by optical lattices and initiated in the Mott insulator phase. In particular, we have been interested in the simulation and study of three-spin interactions conveniently obtained in a lattice with equilateral triangular structure. They appear by a perturbation expansion to the third order with respect to the tunnelling transitions of the atoms when the dominant interactions are collisions of atoms within the same site. Among the models presented here is the $\sigma_i^z \sigma_{i+1}^z \sigma_{i+2}^z$ interaction as well as interactions that explicitly break chiral symmetry. These models exhibit degeneracy in their ground state and undergo a variety of quantum phase transitions that can also be viewed as phases of the initial Mott insulator [25]. The effect of these terms will eventually become significant with the advance of experimental techniques.

The possibility to externally control most of the parameters of the effective Hamiltonians at will qualifies cold atom technology as a unique setup to study exotic systems such as chiral spin systems, fractional quantum Hall systems or systems that exhibit high-T_c superconductivity [21,26]. In addition, suitable applications have been presented within the realm of quantum computation [27] where three-qubit gates can be straightforwardly generated from the three-spin interactions. Unique properties related to the criticality behavior of the chain with three-spin cluster

interactions have been analyzed in [15] where the two-point correlations, used traditionally to describe the criticality of a chain, seem to fail to identify long quantum correlations, suitably expressed by particular entanglement measures [28]. It is unadaptable then that optical lattices offer a unique laboratory to simulate condensed matter systems and to probe new properties of great theoretical and technological interest.

5. acknowledgements

This work was supported by the Royal Society.

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